HEAT FLOW BY PHONONS IN GENERALIZED ELECTRON TRANSPORT MODEL FOR MICRO- AND NANOELECTRONICS

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Electrons transfer both charge and heat. Electrons carry most of the heat in metals. In semiconductors electrons carry only a part of the heat but most of the heat is carried by phonons.

The objectives for this report is to give a condensed summary of Generalized electron transport model [1, 2] to describe the phonon heat flux which works at the nanoscale as well as at macroscale for 1D, 2D, and 3D resistors in ballistic, quasi-ballistic, and diffusive linear response regimes.

The phonon heat flux is proportional to the temperature gradient

$$J_{Qx}^{ph} = -\kappa_L \frac{dT}{dx} \, [W/m^2] \tag{1}$$

with coefficient κ_L known as the specific lattice thermal conductivity. Such an exceptional thermal conductor like diamond has $\kappa_L \approx 2 \cdot 10^3 \, W/m \cdot K$ while such a poor thermal conductor like glass has $\kappa_L \approx 1 \, W/m \cdot K$. Note that electrical conductivities of solids vary over more than 20 orders of magnitude, but thermal conductivities of solids vary over a range of only 3 – 4 orders of magnitude. We will see that the same methodology used to describe electron transport can be also used for phonon transport. We will also discuss the differences between electron and phonon transport.

To describe the phonon current we need an expression like for the electron current

$$I = \frac{2q}{h} \int T_{el}(E) M_{el}(E) \left(f_1 - f_2 \right) dE \, . \tag{2}$$

For electrons the states in the contacts were filled according to the equilibrium Fermi functions, but phonons obey Bose statistics, thus the phonon states in the contacts are filled according to the equilibrium Bose – Einstein distribution

$$n_0(\hbar\omega) = \frac{1}{e^{\hbar\omega/kT} - 1} \, . \tag{3}$$

Let temperature for the left and the right contacts are T_1 and T_2. As for the electrons, both contacts are assumed ideal. Thus the phonons that enter a contact are not able to reflect back, and transmission coefficient $T_{ph}(E)$ describes the phonon transmission across the entire channel.

It is easy now to rewrite eqn. (2) to the phonon heat current. Electron energy E we replace to the phonon energy $\hbar\omega$. In the electron current we have charge q moving in the channel, in case of the phonon current the quantum of energy $\hbar\omega$ is moving instead; thus, we replace q in (2) with $\hbar\omega$ and move it inside the integral. The coefficient 2 in (2) reflects the spin degeneracy of an electron. In case of the phonons we remove this coefficient, and instead the number of the phonon polarization states that contribute to the heat flow let us include to the number of the phonon modes $M_{ph}(\hbar\omega)$. Finally, the heat current due to phonons is

$$Q = \frac{1}{h}\int (\hbar\omega) T_{ph}(\hbar\omega) M_{ph}(\hbar\omega)\left(n_1 - n_2\right) d(\hbar\omega) \, .[W] \tag{4}$$

In the linear response regime

$$n_1 - n_2 \approx -\frac{\partial n_0}{\partial T}\Delta T \, , \tag{5}$$

where the derivative according (3)

$$\frac{\partial n_0}{\partial T} = \frac{\hbar\omega}{T}\left(-\frac{\partial n_0}{\partial(\hbar\omega)}\right), \tag{6}$$

with

$$\frac{\partial n_0}{\partial(\hbar\omega)} = \left(-\frac{1}{kT}\right)\frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT}-1)^2} \, . \tag{7}$$

Now eqn (4) for small differences in temperature becomes

$$Q = -K_L \Delta T \, , \tag{8}$$

where the thermal conductance

$$K_L = \frac{k^2 T}{h}\int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega)\left[\left(\frac{\hbar\omega}{kT}\right)^2\left(-\frac{\partial n_0}{\partial(\hbar\omega)}\right)\right] d(\hbar\omega). \tag{9}$$

Equation (8) is simply the Fourier's law stating that heat flows down to a temperature gradient. It is also useful to note that the thermal conductance (9) displays certain similarities with the electrical conductance

$$G = \frac{2q^2}{h}\int T_{el}(E) M_{el}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE \, . \tag{10}$$

The derivative

$$W_{el}(E) \equiv \left(-\frac{\partial f_0}{\partial E}\right) \tag{11}$$

known as the Fermi window function that separating out those conduction modes which only contribute to the electric current. The electron window function is normalized:

$$\int_{-\infty}^{+\infty} \left(-\frac{\partial f_0}{\partial E}\right) dE = 1. \tag{12}$$

In case of phonons the term in square brackets of eqn (9) acts as a window function to specify which modes carry the heat current. After normalization

$$W_{ph}(\hbar\omega) = \frac{3}{\pi^2}\left(\frac{\hbar\omega}{kT}\right)\left(\frac{\partial n_0}{\partial(\hbar\omega)}\right); \tag{13}$$

thus finally

$$K_L = \frac{\pi^2 k^2 T}{3h} \int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega) \tag{14}$$

with

$$g_0 \equiv \pi^2 k^2 T / 3h \approx (9.456 \times 10^{-13}\, W / K^2) T\ , \tag{15}$$

known as the quantum of thermal conductance experimentally observed first in 2000.

Comparing eqns (10) and (14) one can see that the electrical and thermal conductances are similar in structure: both are proportional to corresponding quantum of conductance times an integral over the transmission times the number of modes times a window function.

The thermal broadening functions for electrons and phonons have similar shapes and each has a width of a few *kT*. In case of electrons this function is

$$F_T(x) \equiv \frac{e^x}{\left(e^x + 1\right)^2} \tag{16}$$

with $x \equiv (E - E_F)/kT$. This function for phonons is given by eqn (13) or

$$F_T^{ph}(x) \equiv \frac{3}{\pi^2} \frac{x^2 e^x}{\left(e^x - 1\right)^2} \tag{17}$$

with $x \equiv \hbar\omega / kT$. Both functions are normalized to a unity and shown together on fig. 1.

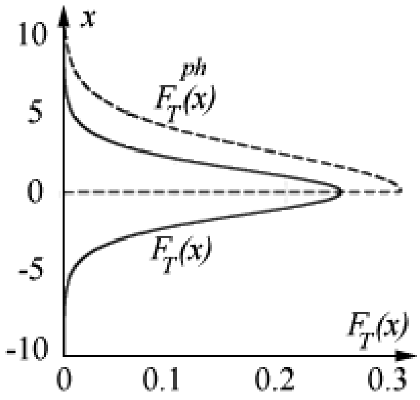

Fig. 1. Broadening function for phonons compared to that of electrons.

Along with the number of modes determined by the dispersion relation, these two window functions play a key role in determining the electrical and thermal conductances.

The thermal conductivity of a large diffusive resistor is a key material property that controls performance of any electronic devices. By analogy with the transmission coefficient for electron transport the phonon transmission

$$T_{ph}(\hbar\omega) = \frac{\lambda_{ph}(\hbar\omega)}{\lambda_{ph}(\hbar\omega) + L}\Big|_{L \gg \lambda_{ph}} \rightarrow \frac{\lambda_{ph}(\hbar\omega)}{L}. \tag{18}$$

It is also obvious that for large 3D conductors the number of phonon modes is proportional to the cross-sectional area of the sample:

$$M_{ph}(\hbar\omega) \propto A, \tag{19}$$

Now let us return to eqn (8) dividing and multiplying it by *A/L*, which immediately gives eqn (1) for the phonon heat flux postulated above

$$\frac{Q}{A} \equiv J_{Qx}^{ph} = -\kappa_L \frac{dT}{dx} \tag{20}$$

with specific lattice thermal conductivity

$$\kappa_L = K_L \frac{L}{A}, \tag{21}$$

or substituting (18) to (14) one for the lattice thermal conductivity finally obtains

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \int \frac{M_{ph}(\hbar\omega)}{A} \lambda_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega). \tag{22}$$

It is useful now to define the average number of phonon modes per cross-sectional area of the conductor that participate in the heat transport

$$\langle M_{ph} / A \rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)\,. \tag{23}$$

Then

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \langle M_{ph} / A \rangle \langle\langle \lambda_{ph} \rangle\rangle, \tag{24}$$

where the average mean-free-path is defined now as

$$\langle\langle \lambda_{ph} \rangle\rangle = \frac{\int \frac{M_{ph}(\hbar\omega)}{A} \lambda_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)}\,. \tag{25}$$

Thus, the couple of the phonon transport equations (20) and (24) corresponds to similar electron transport equations:

$$J_x = \frac{\sigma}{q} \frac{d\left(E_F\right)}{dx}\,, \tag{26}$$

$$\sigma = \frac{2q^2}{h} \langle M_{el} / A \rangle \langle\langle \lambda_{el} \rangle\rangle\,. \tag{27}$$

The thermal conductivity (24) and the electrical conductivity (27) have the same structure. It is always a product of the corresponding quantum of conductance times the number of modes that participate in transport, times the average mean-free-path. These three quantities for phonons will be discussed later.

References

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